

AMENDMENTS TO THE CLAIMS

1-7. (Canceled)

8. (Currently Amended) A computer-implemented method for integrated modeling and simulation of a biological process comprising a plurality of chemical substances, the method comprising:

- (a) constructing, using a suitably programmed computer, a model of the biological process, the constructed model being modified by user commands received through both a graphical user interface and a textual user interface that is separate from the graphical user interface, ~~the textual user interface allowing a user to create a script that automatically edits the constructed model,~~ the constructed model including a first set of data that represents a first state of the plurality of chemical substances and having a layered hierarchy comprising a plurality of hierarchical levels, at least one hierarchical level formed by creating at least one subsystem in the constructed model, each subsystem formed by representing a plurality of blocks of the model as a single block in the constructed model;
- (b) presenting each hierarchical level in a separate window in the graphical user interface
- ~~(b)~~ (c) simulating, using the suitably programmed computer, the constructed model of the biological process to transform the first set of data into a second set of data representing a second state of the plurality of chemical substances in the modeled biological process during a simulation of the biological process; and
- ~~(c)~~ (d) automatically refining, using the suitably programmed computer, the constructed model based on the simulation; and
- (e) displaying one or more results of simulating the constructed model of the biological process to a user.

9. (Previously Presented) The method of claim 8 wherein (a) comprises constructing a block diagram model of a chemical reaction that is part of the biological process.

10. (Original) The method of claim 9 wherein the block diagram model includes at least one block identifying a set of related chemical reactions that are part of the biological process.

11. (Previously Presented) The method of claim 8 wherein (a) further comprises:

- (i) providing the graphical user interface for accepting user commands and data;
 - (ii) receiving, via the provided graphical user interface, user commands and data;
- and
- (iii) constructing, using the received user commands and data, a model of the biological process.

12. (Previously Presented) The method of claim 8 wherein (b) comprises generating, using the constructed model of the biological process, dynamic behavior of the modeled biological process using a stochastic computational model.

13-14. (Canceled)

15. (Currently Amended) A computer-readable medium storing computer-executable instructions for integrated modeling and simulation of a biological process, the medium storing one or more instructions for:

constructing a model of the biological process, wherein the constructed model is modified by user commands received through both a graphical user interface and a textual user interface that is separate from the graphical user interface, ~~the textual user interface allowing a user to create a script that automatically edits the constructed model~~ the constructed model having a layered hierarchy comprising a plurality of hierarchical levels, at least one hierarchical level formed by creating at least one subsystem in the constructed

model, each subsystem formed by representing a plurality of blocks of the model as a single block in the constructed model;

presenting each hierarchical level in a separate window in the graphical user interface;
generating, using the constructed model of the biological process, an expected output of the modeled biological process during the simulation of the biological process; and
automatically refining the constructed model based on the expected output; and
displaying one or more results of the simulation of the biological process to a user.

16. (Previously Presented) The article of manufacture of claim 15 wherein the one or more computer-readable instructions for constructing a model of the biological process comprise one or more computer-readable instructions for constructing a block diagram model of a biological process.

17. (Previously Presented) The article of manufacture of claim 16 wherein the one or more computer-readable instructions for constructing a block diagram model of the biological process include one or more computer-readable instructions for constructing at least one block identifying a set of related chemical reactions.

18. (Previously Presented) The article of manufacture of claim 15 wherein the one or more computer-readable instructions for generating a dynamic behavior of the modeled biological process comprise one or more computer-readable instructions for generating an expected result of the modeled biological process using a stochastic computational model.

19. (Canceled)

20. (Currently Amended) A computer-implemented method for integrated modeling and simulation of a biological process comprising a plurality of chemical substances, the method comprising:

(a) constructing, using a suitably programmed computer, a model of a biochemical process in a modeling component, the constructed model including a first set of data that represents a first state of the plurality of chemical substances, the constructed model being modified by user commands received through both a graphical user interface and a textual user interface that is separate from the graphical user interface, ~~wherein the textual user interface automatically prompts a second user input in response to a first user input received through the graphical user interface~~ the constructed model having a layered hierarchy comprising a plurality of hierarchical levels, at least one hierarchical level formed by creating at least one subsystem in the constructed model, each subsystem formed by representing a plurality of blocks of the model as a single block in the constructed model;

(b) presenting each hierarchical level in a separate window in the graphical user interface;

(~~b~~c) analyzing, using the suitably programmed computer, a simulation of the constructed model of the biological process to generate a second set of data representing a second state of the plurality of chemical substances in the modeled biological process; and

(~~e~~d) transmitting, using the suitably programmed computer, the second set of data to the modeling component, wherein the constructed model is automatically refined based on the simulation of the constructed model of the biological process; and

(~~e~~) displaying one or more results of the simulation of the constructed model of the biological process to a user.

21. (Canceled)

22. (Previously Presented) The method of claim 20 wherein (b) comprises analyzing the constructed model of the biological process using sensitivity analysis.

23-25. (Canceled)

26. (Currently Amended) A computer-implemented system for integrated modeling and simulation of a chemical reaction comprising:

a processor configured to process:

a modeling component for constructing a model of a chemical substance, the constructed model including a first set of data that represents a first state of the chemical substance, the constructed model being modified by user commands received through both a graphical user interface and a textual user interface that is separate from the graphical user interface, the constructed model having a layered hierarchy comprising a plurality of hierarchical levels, at least one hierarchical level formed by creating at least one subsystem in the constructed model, each subsystem formed by representing a plurality of blocks of the model as a single block in the constructed model;

~~wherein the textual user interface automatically prompts a second user input in response to a first user input received through the graphical user interface, [[:]] and~~

a simulation engine in communication with the modeling component, the simulation engine accepting as input the constructed model of the chemical substance and transforming the first set of data into a second set of data representing a second state of the chemical substance, the constructed model being automatically refined based on the first and second sets of data to create a refined model; and

a display for displaying each hierarchical level in a separate window in the graphical user interface.

27. (Original) The system of claim 26 wherein the modeling component comprises an environment for construction of a block diagram model of a chemical reaction.

28. (Original) The system of claim 27 wherein the modeling component further includes at least one block identifying a set of related chemical reactions.

29. (Original) The system of claim 26 wherein the modeling component accepts user commands and input for constructing the model of the chemical reaction.

30. (Previously Presented) The system of claim 26 wherein the simulation engine generates the expected output using a stochastic computational model.

31-32. (Canceled)

33. (Currently Amended) A computer-implemented method for integrated modeling and simulation of chemical reactions, the method comprising:

(a) constructing, using a suitably programmed computer, a model of a chemical substance, the constructed model including a first set of data that represents a first state of the chemical substance, the constructed model being modified by user commands received through both a graphical user interface and a textual user interface that is separate from the graphical user interface, the constructed model having a layered hierarchy comprising a plurality of hierarchical levels, at least one hierarchical level formed by creating at least one subsystem in the constructed model, each subsystem formed by representing a plurality of blocks of the model as a single block in the constructed model;

(b) presenting each hierarchical level in a separate window in the graphical user interface;

~~the textual user interface allowing a user to create a script that automatically edits the constructed model;~~

(~~b~~c) simulating, using the suitably programmed computer, the constructed model of the chemical substance to transform the first set of data into a second set of data representing a second state of the chemical substance; and

(e~~d~~) automatically refining, using the suitably programmed computer, the constructed model based on the simulation to create a refined model; and

(e) displaying the refined model to a user.

34. (Previously Presented) The method of claim 33 wherein (a) comprises constructing a block diagram model of a chemical reaction.

35. (Original) The method of claim 34 wherein the block diagram model includes at least one block identifying a set of related chemical reactions.

36. (Previously Presented) The method of claim 33 wherein (a) comprises:

- (i) providing a graphical user interface for accepting user commands and data;
- (ii) receiving, via the provided user interface, user commands and data; and
- (iii) constructing, using the received user commands and data, a model of the chemical reaction.

37. (Previously Presented) The method of claim 33 wherein (b) comprises generating, using the constructed model of the chemical reaction, an expected output of the modeled chemical reaction using a stochastic computational model.

38-39. (Canceled)

40. (Currently Amended) A computer-readable medium storing computer-executable instructions for integrated modeling of chemical reactions, the medium comprising instructions for:

constructing a model of a chemical reaction, wherein the constructed model is modified by user commands received through both a graphical user interface and a textual user interface that is separate from the graphical user interface, ~~the textual user interface allowing a user to create a script that automatically edits the constructed model~~ the constructed model having a layered hierarchy comprising a plurality of hierarchical levels, at least one hierarchical level formed by creating at least one subsystem in the constructed model, each subsystem formed by representing a plurality of blocks of the model as a single block in the constructed model;

presenting each hierarchical level in a separate window in the graphical user interface;
generating, using the constructed model of the chemical reaction, an expected output of the modeled chemical reaction; ~~and~~

automatically refining the constructed model based on the expected output to created a refined model; and

displaying the refined model to a user.

41. (Previously Presented) The article of manufacture of claim 40 wherein the one or more computer-readable instructions for constructing a model of the chemical reaction comprise one or more computer-readable instructions for constructing a block diagram model of a chemical reaction.

42. (Previously Presented) The article of manufacture of claim 41 wherein the one or more computer-readable instructions for constructing a block diagram model of the chemical reaction include one or more computer-readable instructions for constructing at least one block identifying a set of related chemical reactions.

43. (Previously Presented) The article of manufacture of claim 40 wherein one or more computer-readable instructions for generating an expected result of the modeled chemical reaction comprise one or more computer-readable instructions for generating an expected result of the modeled chemical reaction using a stochastic computational model.

44. (Canceled)

45. (Currently Amended) A computer-implemented method for integrated modeling of chemical reactions, the method comprising:

(a) constructing, using a suitably programmed computer, a model of a chemical substance, the constructed model including a first set of data that represents a first state of the chemical substance, the constructed model being modified by user commands received through both a graphical user interface and a textual user interface that is separate from the graphical user interface, the constructed model having a layered hierarchy comprising a plurality of hierarchical levels, at least one hierarchical level formed by creating at least one subsystem in the constructed model, each subsystem formed by representing a plurality of blocks of the model as a single block in the constructed model;

(b) presenting each hierarchical level in a separate window in the graphical user interface;

~~the graphical user interface allowing a user to create a script that automatically edits the constructed model;~~

(bc) analyzing, using the suitably programmed computer, simulation of the constructed model of the chemical substance to generate a second set of data representing a second state of the chemical substance; and

(ed) transmitting, using the suitably programmed computer, the second set of data to the modeling environment, wherein the constructed model is automatically refined based on the simulation of the constructed model of the chemical substance to create a refined model; and

(e) displaying the refined model to a user.

46. (Canceled)

47. (Previously Presented) The method of claim 45 wherein (b) comprises analyzing the constructed model of the chemical reaction using sensitivity analysis.

48-51: (Canceled)

52. (Previously Presented) The method of claim 8 further comprising annotating the model to add user-provided annotations.

53. (Previously Presented) The method of claim 8 wherein (a) comprises automatically connecting elements of the model using an auto-connection tool.

54. (Previously Presented) The method of claim 8 further comprising providing a tabular view of the model and a graphical view of the model to the user.

55. (Previously Presented) The method of claim 9 wherein (a) comprises constructing the block diagram to include a virtual block that is provided for graphical convenience but that plays no role in the semantics of the model.

56. (Previously Presented) The method of claim 8 further comprising generating a report regarding the model.

57. (Previously Presented) The method of claim 8 further comprising generating code for executing the model.

58. (Previously Presented) The method of claim 57 further comprising distributing the code for distributed execution.

59. (Previously Presented) The method of claim 8 further comprising creating a library from a portion of the model for reuse in another model.

60. (Previously Presented) The method of claim 8 wherein (a) comprises using a knowledge base of chemical reactions in constructing the model.

61. (Previously Presented) The method of claim 8 wherein (a) comprises enabling a user to specify a rapidity of at least one of chemical reactions of the biological process.

62. (Previously Presented) The method of claim 8 wherein the (a) comprises programmatically determining a graphical display that represents the model.

63. (Previously Presented) The method of claim 8 wherein (a) comprises constructing a conditionally executed sub-section that is executed upon satisfaction of a condition.

64. (Previously Presented) The system of claim 26 further comprising an annotation tool for enabling a user to add annotations to the model.

65. (Previously Presented) The system of claim 26 further comprising an auto-connection tool for automatically connecting elements of the model.

66. (Previously Presented) The system of claim 26 further comprising a graphical view of the model and a tabular view of the model that are viewable by user.

67. (Previously Presented) The system of claim 27 wherein the block diagram model contains a virtual block that is provided for graphical convenience but plays no role in semantics of the model.

68-76. (Canceled)

77. (Previously Presented) The article of manufacture of claim 40 further comprising one or more computer-readable instructions for annotating the model to add user-provided annotations.

78. (Previously Presented) The article of manufacture of claim 40 further comprising one or more computer-readable instructions for automatically connecting elements of the model.

79. (Previously Presented) The article of manufacture of claim 40 further comprising one or more computer-readable instructions for providing a tabular view of the model and a graphical view of the model.

80. (Previously Presented) The article of manufacture of claim 41 wherein the one or more computer-readable instructions for constructing a block diagram model of the chemical reaction include one or more computer-readable instructions for constructing at least one block identifying a set of related chemical reactions.

81. (Previously Presented) The article of manufacture of claim 41 wherein the one or more computer-readable instructions for constructing the model of the chemical reactions construct the block diagram to include a virtual block that is provided for graphical convenience but plays no role in semantics of the model.

82. (Previously Presented) The article of manufacture of claim 40 further comprising one or more computer-readable instructions for generating code for executing the model.

83. (Previously Presented) The article of manufacture of claim 79 further comprising one or more computer-readable instructions for distributing the code that is generated for distributed execution.

84. (Previously Presented) The article of manufacture of claim 40 wherein the one or more computer-readable instructions for constructing the model of the chemical reactions use a knowledge base of chemical reactions to construct the model.

85. (Previously Presented) The article of manufacture of claim 40 wherein the one or more computer-readable instructions for constructing the model of the chemical reactions enable a user to specify a rapidity of at least one of the chemical reactions.

86. (Previously Presented) The article of manufacture of claim 40 wherein the one or more computer-readable instructions for constructing the model of the chemical reactions determine a graphical display for representing the model.

87. (Previously Presented) The article of manufacture of claim 40 wherein the one or more computer-readable instructions for constructing the model of the chemical reactions construct the model to include a conditional sub-section that executed upon satisfaction of a condition.